

What is claimed is:

Claims

1. A method for use in deriving a chemical structure diagram,
comprising:

5 identifying, from a connection table for a chemical structure, an instance
of chemical structural symmetry in the chemical structure; and

expressing the instance of chemical structural symmetry in the chemical
structure diagram.

10 2. A method for use in deriving a chemical structure diagram,
comprising:

determining, from a first chemical structure diagram, a force term for
increasing diagrammatic symmetry within the first chemical structure diagram;
and

15 applying the force term in a derivation of a second chemical structure
diagram from the first chemical structure diagram, the second chemical structure
diagram having more diagrammatic symmetry than the first chemical structure
diagram.

3. A method for use in deriving a chemical structure diagram,
comprising:

determining, from a first chemical structure diagram, a parameter for use
in producing the shape of an addition to the first chemical structure diagram;

5 producing the shape of the addition based on the parameter; and
 producing a second chemical structure diagram by adding the addition to
the first chemical structure diagram.

4. A method for use in deriving a chemical structure diagram,
10 comprising:

determining a first rectangle that defines a first portion of an available
layout area, the first rectangle being of a sufficient size to enclose a first chemical
structure diagram;

determining a second rectangle that defines a second portion of an
15 available layout area, the second portion being non-overlapping with the first
portion, the second rectangle being of a sufficient size to enclose a second
chemical structure diagram; and

positioning the first and second chemical structure diagrams within the
first and second portions, respectively.

5. A system for use in deriving a chemical structure diagram, comprising:
an identifier identifying, from a connection table for a chemical structure,
an instance of chemical structural symmetry in the chemical structure; and
an expressor expressing the instance of chemical structural symmetry in
5 the chemical structure diagram.

6. A system for use in deriving a chemical structure diagram, comprising:
a determiner determining, from a first chemical structure diagram, a force
term for increasing diagrammatic symmetry within the first chemical structure
10 diagram; and

an applicator applying the force term in a derivation of a second chemical
structure diagram from the first chemical structure diagram, the second chemical
structure diagram having more diagrammatic symmetry than the first chemical
structure diagram.

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7. A system for use in deriving a chemical structure diagram, comprising:
a determiner determining, from a first chemical structure diagram, a
parameter for use in producing the shape of an addition to the first chemical
structure diagram; and

a producer producing the shape of the addition based on the parameter and producing a second chemical structure diagram by adding the addition to the first chemical structure diagram.

5 8. A system for use in deriving a chemical structure diagram, comprising:

a determiner determining a first rectangle that defines a first portion of an available layout area, the first rectangle being of a sufficient size to enclose a first chemical structure diagram, the determiner determining a second rectangle that defines a second portion of an available layout area, the second portion
10 being non-overlapping with the first portion, the second rectangle being of a sufficient size to enclose a second chemical structure diagram; and

a positioner positioning the first and second chemical structure diagrams within the first and second portions, respectively.

15 9. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

identify, from a connection table for a chemical structure, an instance of
20 chemical structural symmetry in the chemical structure; and

express the instance of chemical structural symmetry in the chemical structure diagram.

10. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

determine, from a first chemical structure diagram, a force term for increasing diagrammatic symmetry within the first chemical structure diagram;

and

apply the force term in a derivation of a second chemical structure diagram from the first chemical structure diagram, the second chemical structure diagram having more diagrammatic symmetry than the first chemical structure diagram.

11. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

determine, from a first chemical structure diagram, a parameter for use in producing the shape of an addition to the first chemical structure diagram;

produce the shape of the addition based on the parameter; and

produce a second chemical structure diagram by adding the addition to

5 the first chemical structure diagram.

12. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the

10 instructions causing the system to:

determine a first rectangle that defines a first portion of an available layout area, the first rectangle being of a sufficient size to enclose a first chemical structure diagram;

determine a second rectangle that defines a second portion of an available
15 layout area, the second portion being non-overlapping with the first portion, the second rectangle being of a sufficient size to enclose a second chemical structure diagram; and

position the first and second chemical structure diagrams within the first and second portions, respectively.